Quantum Theory with Many Degrees of Freedom from Monte Carlo Hamiltonian

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With our recently proposed effective Hamiltonian via Monte Carlo, we are able to compute low energy physics of quantum systems. The advantage is that we can obtain not only the spectrum of ground and excited states, but also wave functions. The previous work has shown the success of this method in (1+1)-dimensional quantum mechanical systems. In this work we apply it to higher dimensional systems.

1. Introduction

Monte Carlo (MC) method with importance sampling is an excellent technique to calculate high dimensional integrals, and has successfully been applied to Lagrangian lattice gauge theory. Recently, we proposed an algorithm to compute the MC Hamiltonian [1]. The advantage, in comparison with the standard Lagrangian MC approach, is that one can obtain not only the spectrum of ground and excited states, but also the wave functions. The method has been tested in quantum mechanics (QM) in 1+1 dimensions, where the exact results were reproduced with high precision [1–3]. In this paper, we apply this algorithm to QM in 2+1 dimensions. The motivation is as follows. (a) A number of algorithms for solving the Schrödinger equation in lower dimensions (e.g. Runge-Kutta) do not work in 2+1 dimensions. Our method works in 2+1 dimensions, it is likely to work also in higher dimensions. (b) The ultimate goal of the algorithm is to study structure function, the S matrix, QCD at finite density as well as systems with many degrees of freedom. QM in 2+1 dimensions is a simple example.

2. Algorithm

Let's review briefly the basic ideas [1]. According to Feynman's path integral approach to QM, the (imaginary time) transition amplitude between an initial state at position x_i, and time t_i, and final state at x_f, t_f is related to the Hamiltonian H by

$$< x_f, t_f | x_i, t_i > = < x_f | e^{-H(t_f - t_i)/\hbar} | x_i >$$

$$= \sum_{\nu=1}^{\infty} < x_f | E_\nu > e^{-E_\nu T/\hbar} < E_\nu | x_i >, \qquad (1)$$

where $T = t_f - t_i$. The starting point of our method, as described in detail in [1] is to construct an effective Hamiltonian H_{eff} (finite $N \times N$ matrix) by

$$< x_f | e^{-H(t_f - t_i)/\hbar} | x_i > \approx < x_f | e^{-H_{eff} T/\hbar} | x_i >$$

$$= \sum_{\nu=1}^{N} < x_f | E_\nu^{eff} > e^{-E_\nu^{eff} T/\hbar} < E_\nu^{eff} | x_i > . \qquad (2)$$

H_{eff} can be found by MC simulation using the following procedure:

(a) Discretize the continuous time.
(b) Generate configurations $[x]$ obeying the Boltzmann distribution

$$P(x) = \frac{\exp(-S[x]/\hbar)}{\int [dx] \exp(-S[x]/\hbar)}. \quad (3)$$

(c) Calculate the transition matrix elements

$$M_{fi} = < x_f | e^{-H_{eff} T/\hbar} | x_i > \quad (4)$$

between N discrete x_i points and N x_f points. Note that the matrix M is symmetric.
(d) Diagonalize M by a unitary transformation

$$M = U^\dagger D U, \quad (5)$$

where $D = diag(e^{-E_1^{eff} T/\hbar}, ..., e^{-E_N^{eff} T/\hbar})$. Steps (a) and (b) are the same as the standard MC method. Step (c) is the essential ingredient of our method, from which we can construct H_{eff}, and obtain the eigenvalues E_ν^{eff} and wavefunction $|E_\nu^{eff}>$ through step (d). Once the spectrum and wave functions are available, all physical information can be retrieved. Since the theory described by H is now approximated by a theory described by a finite matrix H_{eff}, the physics of H and H_{eff} might be quite different at high energy. Therefore we expect that we can only reproduce the low energy physics of the system. This is good enough for our purpose.

3. Results

We consider the following examples in $D = 2$:

3.1. Uncoupled harmonic oscillator

The Euclidean action is given by

$$S = \int_0^T dt \left[\frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m\omega^2}{2}(x^2 + y^2) \right]. \quad (6)$$

The spectrum is degenerate and exactly known:

$$E_{n_1,n_2} = \omega\hbar(n_1 + n_2 + 1), \; n_1, n_2 = 0, 1, 2, \ldots \quad (7)$$

3.2. Coupled harmonic oscillator

The Euclidean action is given by

$$S = \int_0^T dt \left[\frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m\omega^2}{2}(x^2 + y^2) + \lambda xy \right],$$

$$\text{for } 0 < \lambda < \mathrm{m}\omega^2. \quad (8)$$

The spectrum is also exactly known:

$$E_{n_1,n_2} = \omega_1\hbar(n_1 + \frac{1}{2}) + \omega_2\hbar(n_2 + \frac{1}{2}),$$

$$n_1, n_2 = 0, 1, 2, \ldots, \quad (9)$$

where $\omega_1 = \sqrt{\omega^2 + \frac{\lambda}{m}}$ and $\omega_2 = \sqrt{\omega^2 - \frac{\lambda}{m}}$.

3.3. Summary

Tabs. 1 and 2 compare the spectrum from H_{eff} with the exact results. Figs. 1-4 show the first two wave functions. They are in very good agreement with the exact ones, at least in the low energy domain. In Ref. [4], more results for wave functions of higher execited states, and thermodynamical quantities such as the average energy and specific heat, were reported. However, the CPU time is much longer than in 1-dimensional systems. We need to find a better (stochastic) way to select the basis in Hilbert space in step (c) of Sect. 2, before extending the method to quantum field theory. We are curious to see if our method can resolve the long standing problem of QCD at finite density. It is worth mentioning the recent analytical [5] and numerical [6] efforts in Hamiltonian formulation.

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Table 1
Spectrum of *uncoupled* hamonic oscilator.

n_1, n_2	$E^{MC}_{n_1 n_2}$	$E^{Exact}_{n_1 n_2}$
0, 0	0.9975 ± 0.0258	1.0000
0, 1	1.9902 ± 0.0420	2.0000
1, 0	2.0022 ± 0.0468	2.0000
0, 2	2.9499 ± 0.0393	3.0000
2, 0	2.9815 ± 0.0550	3.0000
1, 1	3.0014 ± 0.0546	3.0000
$n_1 + n_2 = 3$	3.9718 ± 0.0496	4.0000
$n_1 + n_2 = 3$	3.9853 ± 0.0626	4.0000
$n_1 + n_2 = 3$	4.0547 ± 0.0611	4.0000
$n_1 + n_2 = 3$	4.0713 ± 0.0851	4.0000

Table 2
Spectrum of *coupled* hamonic oscilator.

n_1, n_2	$E^{MC}_{n_1 n_2}$	$E^{Exact}_{n_1 n_2}$
0, 0	0.9640 ± 0.0245	0.9659
0, 1	1.6693 ± 0.0335	1.6730
1, 0	2.1843 ± 0.0535	2.1907
0, 2	2.3650 ± 0.0363	2.3801
1, 1	2.8818 ± 0.0553	2.8978
0, 3	3.0883 ± 0.0447	3.0872
0, 3	3.0883 ± 0.0447	3.0872
2, 0	3.4049 ± 0.0532	3.4154
1, 2	3.6275 ± 0.0526	3.6049
0, 4	3.7414 ± 0.0327	3.7944

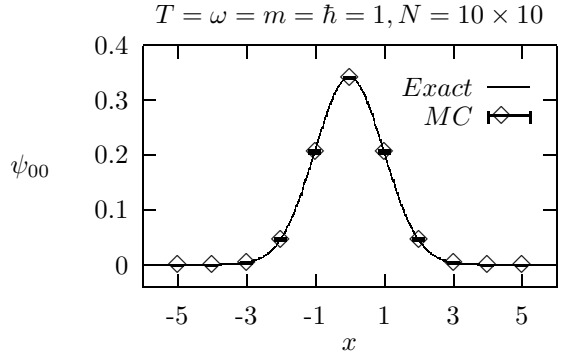

Figure 1. $\psi_{n_1 n_2}(x, y)$ vs. x at $y = -1$ for *uncoupled* harmonic oscillator with $n_1 = n_2 = 0$.

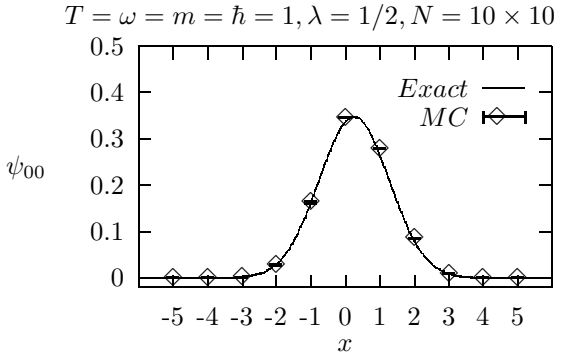

Figure 3. $\psi_{n_1 n_2}(x, y)$ vs. x at $y = -1$ for *coupled* harmonic oscillator with $n_1 = n_2 = 0$.

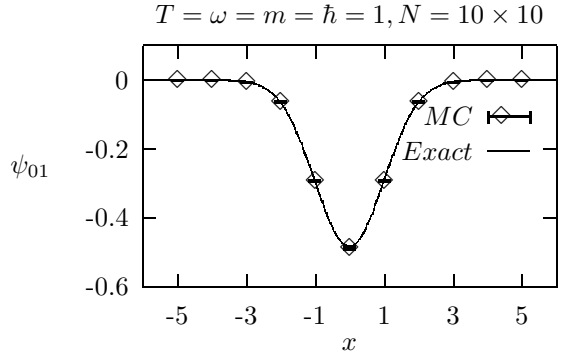

Figure 2. $\psi_{n_1 n_2}(x, y)$ vs. x at $y = -1$ for *uncoupled* harmonic oscillator with $n_1 = 0, n_2 = 1$.

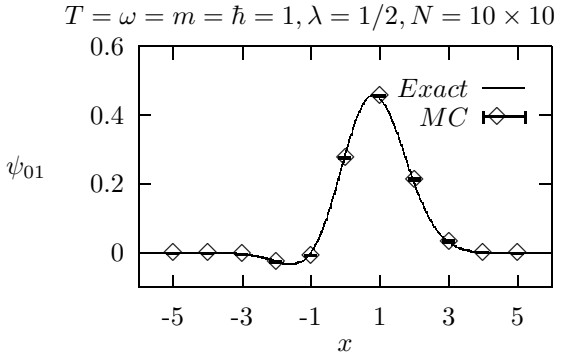

Figure 4. $\psi_{n_1 n_2}(x, y)$ vs. x at $y = -1$ for *coupled* harmonic oscillator with $n_1 = 0, n_2 = 1$.